

**WHAT IS CLAIMED IS:**

1. A heterodiamondoid comprising a diamondoid nucleus selected from a triamantane or higher diamondoid nucleus having at least one of its carbon atoms replaced by a heteroatom.
2. The heterodiamondoid of claim 1 wherein at least one secondary carbon in the diamondoid nucleus is replaced by a heteroatom.
3. The heterodiamondoid of claim 1 wherein at least one tertiary carbon in the diamondoid nucleus is replaced by a heteroatom.
4. The heterodiamondoid of claim 1 comprising one heteroatom.
5. The heterodiamondoid of claim 1 comprising more than one heteroatoms.
6. The heterodiamondoid of claim 1 comprising two or more different heteroatoms.
7. The heterodiamondoid of claim 1 wherein the at least one heteroatoms are independently selected from the IIIB, non-C IVB, VB and VIB atoms in the periodic table of the elements.
8. The heterodiamondoid of claim 7 wherein the at least one heteroatoms are independently selected from the group consisting of the following atoms: Se, As, B, Al, Si, N, P, O and S.
9. A heterodiamondoid of claim 1 wherein the diamondoid nucleus is a triamantane nucleus.
10. A heterodiamondoid of claim 1 wherein the diamondoid nucleus is a higher diamondoid nucleus.

11. A heterodiamondoid of claim 1 wherein at least one of the heteroatoms replacing a carbon atom is an electron-donating heteroatom.
12. The heterodiamondoid of claim 11, wherein the electron-donating heteroatom is a group VB element.
13. The heterodiamondoid of claim 11, wherein the electron-donating heteroatom is selected from the group consisting of nitrogen, phosphorus, and arsenic.
14. The heterodiamondoid of claim 11, which is an aza-diamondoid.
15. The heterodiamondoid of claim 11, wherein the electron-donating heteroatom is  $sp^3$ -hybridized in the diamond lattice.
16. A heterodiamondoid of claim 1 wherein at least one of the heteroatoms replacing a carbon atom is an electron-withdrawing heteroatom.
17. The heterodiamondoid of claim 16, wherein the electron-withdrawing heteroatom is a group IIIB element.
18. The heterodiamondoid of claim 17, wherein the electron-withdrawing heteroatom is selected from the group consisting of boron and aluminum.
19. The heterodiamondoid of claim 18, wherein the electron-withdrawing element is boron.
20. The heterodiamondoid of claim 16, wherein the electron-withdrawing heteroatom occupies a substitutional site on the diamond lattice.
21. The heterodiamondoid of claim 16, wherein the electron-withdrawing heteroatom is  $sp^3$ -hybridized in the diamond lattice.
22. A method of synthesizing an aza-diamondoid, the method comprising:

- a) converting a diamondoid selected from triamantane and the higher diamondoids to a hydroxy-diamondoid;
  - b) preparing an aza-homodiamondoid-ene from the hydroxy-diamondoid;
  - c) preparing an epoxy aza-homodiamondoid from the aza-homodiamondoid-ene; and
  - d) preparing an aza-diamondoid from the epoxy aza-homodiamondoid.
23. A method of synthesizing an aza-diamondoid, the method comprising:
- a) oxidizing a diamondoid selected from triamantane and the higher diamondoids to a keto-diamondoid;
  - b) preparing a fragmented diamondoid-ene carboxylic acid from the keto-diamondoid;
  - c) preparing a fragmented diamondoid-ene acetate from the fragmented diamondoid-ene carboxylic acid;
  - d) preparing a fragmented hydroxy-diamondoid-ene by reducing the fragmented diamondoid-ene acetate;
  - e) preparing a fragmented keto-diamondoid-ene by oxidizing the fragmented hydroxy-diamondoid-ene;
  - f) preparing a fragmented diamondoid=N-OH-ene from the fragmented keto-diamondoid-ene;
  - g) preparing an aza-diamondoid from the fragmented diamondoid=N-OH-ene.
24. A method of preparing heterodiamondoid, the method comprising:
- a) isolating a diamondoid selected from triamantane and the higher diamondoids from a petroleum feedstock;

- b) converting the diamondoid into a heterodiamondoid by substitutionally positioning an electron-donating heteroatom on a diamond crystal lattice position.
- 25. A method of preparing heterodiamondoid, the method comprising:
  - a) isolating a diamondoid selected from triamantane and the higher diamondoids from a petroleum feedstock;
  - b) converting the diamondoid into a heterodiamondoid by substitutionally positioning an electron-withdrawing heteroatom on a diamond crystal lattice position.
- 26. A functionalized heterodiamondoid comprising a heterodiamondoid of claim 1 with one or more covalently-bonded functional groups pendant from its diamondoid nucleus.
- 27. A functionalized heterodiamondoid comprising a heterodiamondoid of claim 8 with one or more covalently-bonded functional groups pendant from its diamondoid nucleus.
- 28. A functionalized heterodiamondoid comprising a heterodiamondoid of claim 10 with one or more covalently-bonded functional groups pendant from its diamondoid nucleus.
- 29. The functionalized heterodiamondoid of claim 26 wherein the one or more functional groups comprise a group selected from the group consisting of halo, thio, oxide, hydroxyl, nitro, sulfonylhalide, sulfonate, phosphine, added alkyl, alkenyl, alkynyl and aryl, with or without substitution.
- 30. A functionalized heterodiamondoid of claim 26 wherein the one or more functional groups comprise a halo.

31. The functionalized heterodiamondoid of claim 26 wherein the one or more functional groups comprise a hydroxide.
32. The functionalized heterodiamondoid of claim 26 wherein the one or more functional groups comprise an oxide.
33. The functionalized heterodiamondoid of claim 26 wherein the one or more functional groups comprise a nitrate.
34. The functionalized heterodiamondoid of claim 26 wherein the one or more functional groups comprise a group selected from the group consisting of haloalkyl; haloalkenyl; haloalkynyl; hydroxyalkyl; heteroaryl; alkylthio; alkoxy; aminoalkyl; aminoalkoxy; heterocycloalkoxy; cycloalkyloxy; aryloxy; heteroaryloxy;  $-C(O)Z$  wherein Z is hydrogen, alkyl, halo, haloalkyl, halothio, amino, monosubstituted amino, disubstituted amino, cycloalkyl, aryl, heteroaryl;  $-CO_2Z$ ;  $-R^7COZ$  wherein  $R^7$  is alkenyl, aminoalkenyl, or haloalkenyl;  $-R^7COOZ$ ;  $-OSO_3H$ ;  $NH_2$ ;  $NHR'$ ;  $NR'R''$ ; and  $N^+R'R''R'''$  wherein  $R'$ ,  $R''$ , and  $R'''$  are independently alkyl, thio, thioalkyl, heteroalkyl, aryl, or heteroaryl;  $R^8NHCOR^9$  wherein  $R^8$  is selected from the group consisting of  $CH_2$ ,  $OCH_2$ ,  $NHCH_2$ ,  $CH_2CH_2$ , and  $OCH_2CH_2$  and  $R^9$  is selected from the group consisting of alkyl, aryl, heteroaryl, aralkyl, and heteroaraylkly; and  $R^{10}CONHR^{11}$  wherein  $R^{10}$  is selected from the group consisting of  $CH_2$ ,  $OCH_2$ ,  $NHCH_2$ ,  $CH_2CH_2$ , and  $OCH_2CH_2$ , and  $R^{11}$  is selected from the group consisting of alkyl, aryl, heteroaryl, aralkyl, and heteroaralkyl.
35. The functionalized heterodiamondoid of claim 26, wherein the one or more functional groups comprise a polymerizable functional group.
36. The heterodiamondoid of claim 1 as a discrete molecule.
37. The heterodiamondoid of claim 1 as a crystal.